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Influence of medium on thermodynamic parameters of conformational conversions of certain partially fixed seven-membered 1,3-heterocycles, as indicated by NMR data

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Abstract

It has been shown that the observed differences in enthalpy and entropy between equilibrium states of seven-membered 1,3-heterocycles contained contributions from the temperature dependence of permittivity of the medium. These contributions are comparable in magnitude to the differences in enthalpy and entropy characterizing the conformational equilibrium in such solvents as chloroform and methylene chloride. The changes in enthalpy difference of the conformers chair ⇄ twist and chair ⇄ boat in these compounds when the medium is changed are in good agreement with reactive field theory. © 1990 Plenum Publishing Corporation.

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